

# Finite-Temperature Signatures of Spin Liquids in Frustrated Hubbard Model

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Finite-temperature properties of the frustrated Hubbard model are theoretically examined by using the recently proposed thermal pure quantum state, which is an unbiased numerical method for finite-temperature calculations. By performing systematic calculations for the frustrated Hubbard model, we show that the geometrical frustration controls the characteristic energy scale of the metal-insulator transitions. We also find the finite-temperature signatures of the quantum spin liquid; vanishing long-range spin correlations and large remaining entropy at low temperatures. We propose that remaining entropy at moderately high temperature is a useful criterion whether the target systems have a chance to be quantum spin liquids at zero temperature.

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*Introduction.*— Strong correlations among particles often induce localization of the particles and resultant charge-gapped states are called Mott insulators. The Mott insulators have been ubiquitously found in a broad range of condensed matter physics such as transition-metal oxides [1], organic compounds [2], and ultra cold atoms [3]. In most of the Mott insulators in solids, time-reversal symmetry-broken phases such as antiferromagnetic phases appear at sufficiently low temperatures. However, if exchange couplings among electrons' spins compete each other because of geometrical frustrations [4], the quantum melting of the magnetic orders leads to new states of matter such as quantum spin liquids. Actually, in the several organic conductors, it has been pointed out that quantum spin liquids appear [5–7]. It has been one of the hottest issues of the modern condensed matter physics to clarify how the interplay of strong electronic correlations and the geometrical frustration induces the quantum spin liquids [8].

The two-dimensional Hubbard model with geometrical frustrations, which has the nearest-neighbor (next-nearest-neighbor) hopping  $t$  ( $t'$ ) and on-site Coulomb interaction  $U$  (details are defined in Eq. (1) later) is one of the simplest theoretical model that describes competition and cooperation of the strong electronic correlations and the geometrical frustrations. In this model, due to the next-nearest neighbor hopping  $t'$ , which induces the next-nearest neighbor antiferromagnetic interactions, as illustrated in the inset of Fig. 1, the competition between two magnetic phases occurs: a simple Néel state becomes stable for small  $t'$  while a stripe state becomes stable for large  $t'$  region ( $t'/t \sim 1$ ). Several theoretical calculations for the ground states of the frustrated Hubbard model have been done thus far [9–11] and most of the calculations suggest that quantum spin liquid states appear around the intermediate region.

In the strong coupling limit, the low-energy prop-

erties of the frustrated Hubbard model are effectively described by the frustrated ( $J_1$ - $J_2$ ) Heisenberg model ( $J_1 \sim 4t^2/U$ ,  $J_2 \sim 4t'^2/U$ ). In the  $J_1$ - $J_2$  Heisenberg model, intensive highly-accurate numerical simulations reveal that the quantum spin liquid appears between the Néel and stripe states [12–15]. In spite of the huge amount of the studies on the frustrated Hubbard model and  $J_1$ - $J_2$  Heisenberg model, there are few unbiased theoretical studies on the finite-temperature properties that are accessible in experiments because of a lack of efficient theoretical methods.

Recently, an efficient unbiased numerical method for calculating finite-temperature properties in quantum systems is proposed by Sugiura and Shimizu [16]. In this method, by explicitly constructing the thermal pure quantum (TPQ) state, it is shown that thermodynamic properties such as energy as well as the correlation functions are accurately given as expectation values taken with *one* TPQ state for sufficiently large system sizes. This method enables us to calculate the finite-temperature properties *without* ensemble average. Therefore, we can perform the unbiased finite-temperature calculations for a large system size to which full diagonalization method is almost inapplicable. Here, note that, in the pioneering works [17–19], the finite-temperature observables were already calculated by replacing ensemble average with random sampling of wave functions.

In this Letter, by using the TPQ method, we systematically study finite-temperature properties of the frustrated Hubbard model, which is a prototypical system where the competition between the geometrical frustrations and the strong electronic correlations plays a crucial role. From the unbiased and systematic calculations, we clarify impacts of the geometrical frustrations on the Mott transitions and find the finite-temperature signatures of quantum spin liquids. We also propose an ex-

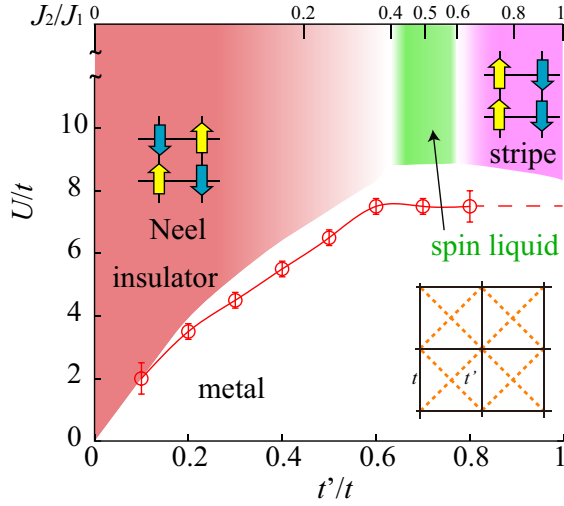


FIG. 1: (color online). Phase diagram for frustrated Hubbard model in comparison with strong-coupling-limit phase diagram. The phase boundary separating insulating and metallic ground states is determined by maxima of  $\chi_D$  (see main article) as a function of on-site Coulomb repulsion  $U$ . Spin liquid may appear between Néel and stripe magnetic orders in the strong coupling region. In the inset, lattice structure used in this study is shown. The nearest-neighbor hopping (next-nearest-neighbor) hopping is represented by  $t$  ( $t'$ ).

perimental criterion of closeness to the spin liquid phase: Finite-temperature entropy at moderately high temperatures significantly correlates with closeness to the spin liquid phase. Experimental searches for spin liquids have so far focused on setting up an *alibi* of spontaneous symmetry breakings down to ultra-low temperatures. However, we reveal that, even at moderately high temperatures  $T \sim t/10$ , it becomes clear whether the target system has chance to be a spin liquid at zero temperature.

*Model and Methods.*— We study the  $t$ - $t'$  Hubbard model on a square lattice (see Fig. 1) defined as

$$\hat{\mathcal{H}} = -t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) is a creation (annihilation) operator of an electron with spin  $\sigma$  at  $i$ th site. The first (second) term describes the hopping of electrons between the nearest-neighbor (next-nearest-neighbor) sites  $\langle i, j \rangle$  ( $\langle\langle i, j \rangle\rangle$ ) on the square lattice, and the third term represents the onsite Coulomb interactions ( $U > 0$ ). In the following, we focus on the half filling, i.e., the filling is given by  $n = N_s^{-1} \sum_{i\sigma} \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle = 1$  ( $N_s = L \times L$  is the system size). To reduce the numerical cost, we only consider the total  $S^z = 0$  space, i.e.,  $S_{\text{total}}^z = \sum_i S_i^z = 0$ . We employ a  $4 \times 4$  cluster with a periodic boundary condition in the rest of the present Letter.

In the micro-canonical TPQ method [16], by multiplying  $(l - \hat{\mathcal{H}}/N_s)$  to random vector  $|\psi_{\text{rand}}\rangle$ , we numerically generate the TPQ state. Here,  $l$  is constant that is larger than the maximum eigenvalue of  $\hat{\mathcal{H}}/N_s$ . The  $k$ th TPQ state is recursively defined as

$$|\psi_k\rangle \equiv \frac{(l - \hat{\mathcal{H}}/N_s)|\psi_{k-1}\rangle}{|(l - \hat{\mathcal{H}}/N_s)|\psi_{k-1}\rangle|} \quad (2)$$

with  $|\psi_0\rangle = |\psi_{\text{rand}}\rangle$ . It is shown that the temperature  $T_k$  corresponding to the  $k$ th TPQ state is estimated from the  $k$ th internal energy  $u_k = \langle \psi_k | \hat{\mathcal{H}} | \psi_k \rangle / N_s$  within the accuracy of  $O(1/N_s)$ , as  $\beta_k = 1/k_B T_k = 2k/N_s(l - u_k) + O(1/N_s)$ , where  $k_B$  is the Boltzmann constant and we take  $k_B = 1$  in this Letter. It is shown that physical properties at  $T = T_k$  can be calculated as the expectation value taken with respect to  $|\psi_k\rangle$ , i.e.,  $\langle \hat{A} \rangle_{T=T_k} = \langle \psi_k | \hat{A} | \psi_k \rangle + O(1/N_s)$ . To estimate the finite-size error, we typically perform five runs initiated with different  $|\psi_{\text{rand}}\rangle$  and regard its standard deviations as error bars.

*Finite-temperature physical quantities in Hubbard models.*— We first show the results of the finite- $T$  calculations for  $t'/t = 0.5$  as an example of weakly frustrated Hubbard models. The ground state is expected to be Néel state for  $t'/t = 0.5$ . Figure 2 (a) shows that temperature dependence of the specific heat  $C/N_s$ , which is given by  $C/N_s = (\langle \hat{\mathcal{H}}^2 \rangle - \langle \hat{\mathcal{H}} \rangle^2) / (N_s T^2)$ . The specific heat has a single peak for  $U/t = 4$  as a function of  $T$  while double-peak structures [20] are universal at strong-coupling regions of the Hubbard-type models irrespective of dimensionality [21–24].

The high-temperature peak of  $C$  is generated by the charge degrees of freedom [20, 25] whose energy scale is determined by  $U$ , as confirmed later by the peak temperatures insensitive to  $t'$  shown in Fig. 4(c). Below the peak temperature, the Mott gap opens and charge degrees of freedom begin to freeze. In other words, below the peak temperature, electrons begin to feel the on-site repulsion  $U$  and double occupancy, which is measured by  $D = N_s^{-1} \sum_{i=1, N_s} \langle n_{i\uparrow} n_{i\downarrow} \rangle$ , is gradually prohibited.

We show temperature dependence of the double occupancy in Fig. 2 (b). Our simulation shows non-monotonic temperature dependence of  $D$  from weak to strong coupling region, i.e.,  $D$  has the minimum around  $T/t \sim 1$ . We note that this non-monotonic behavior is universal one and observed in a wide range of Hubbard-type models [26–29]. The non-monotonic temperature dependence is explained by the development of antiferromagnetic correlations: The antiferromagnetic correlations exclude high-spin states such as triplet states that have larger probability of parallel adjacent spins compared to the singlet state. Because the larger probability of the parallel adjacent spins decreases the probability of the on-site anti-parallel spins (namely, double occupancy), high-spin states generally have smaller double occupancy compared to the singlet states. Therefore, the exclusion

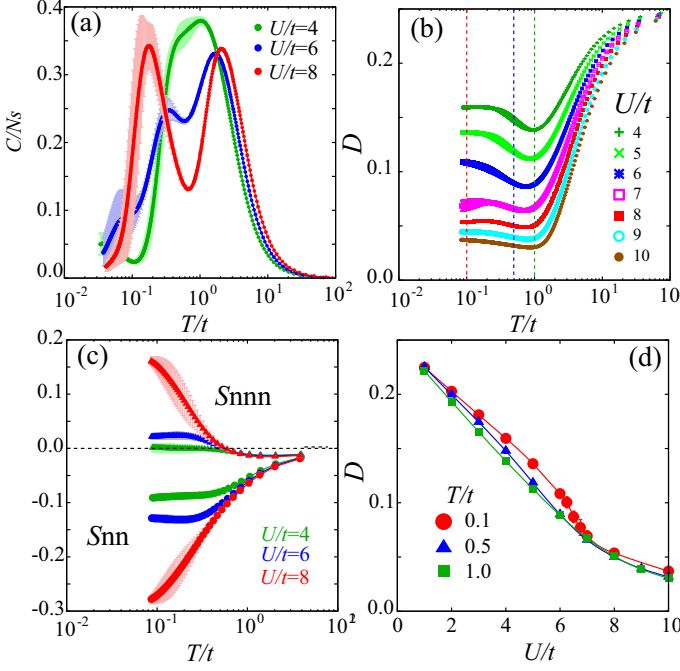


FIG. 2: (color online). (a) Temperature dependence of the specific heat. Error bars are shown as shaded regions. (b) Temperature dependence of double occupancy  $D$  for several  $U$ . Irrespective of interaction strength, we find the non-monotonic temperature dependence of  $D$ . (c) Temperature dependence of the nearest-neighbor (next-nearest-neighbor) spin correlation  $S_{nn}$  ( $S_{nnn}$ ). (d) Interaction ( $U$ ) dependence of  $D$  for  $T/t = 1.0, 0.5, 0.1$ . By lowering temperature, we can see the signature of the finite-temperature Mott transition.

of the high-spin states increases the double occupancy at low temperature.

The low-temperature peak of the specific heat, in contrast to the high-temperature peak, is induced by spin degrees of freedom. The low-temperature peak signals development of antiferromagnetic correlations as shown in Fig. 2 (c), which corresponds to an increase in  $D$  at low temperatures as discussed above. The peak temperature becomes lower as  $U$  increases, as is manifest in Fig. 2 (a), which is consistent with the characteristic energy scale of the spin-degrees of freedom at the strong coupling limit given by the effective superexchange  $J_1 \sim 4t^2/U$ . To examine the energy scale, we show the temperature dependence of the nearest-neighbor (nn) and next-nearest-neighbor (nnn) spin correlations in Fig. 2 (c), which is defined as  $S_p = 1/(z_p N_s) \sum_{i=1}^{N_s} \sum_{\mu} \mathbf{S}_i \cdot \mathbf{S}_{i+e_\mu}$ , where  $p=nn$  or  $nnn$  and accordingly,  $e_\mu$  runs over nn or nnn sites, and  $z_p$  represents the coordination number for nn or nnn sites. As it is expected, the spin correlations develop around the low-temperature peak of the specific heat. The two emergent energy scales corresponding to spin and charge degrees of freedom in the strong coupling re-

gion are indeed identified as origin of two-peak structure of the specific heat for  $U/t \gtrsim 6$  while separation of these energy scales may not be clear in excitation spectra [30].

*Impact of geometrical frustration on metal-insulator transitions.*— To examine the signature of the finite-temperature Mott transitions, we calculate the  $U$ -dependence of  $D$  for several temperatures as shown in Fig. 2 (d). By lowering the temperatures, we find the slope of  $D$  becomes steep. Since the slope of  $D$  diverges at the finite-temperature Mott critical end point [31], this behavior is the signature of the finite-temperature Mott critical point.

To see the  $t'$  dependence of the critical temperatures of the Mott transitions, we calculate the  $U$  dependence of  $D$  for several different  $t'$  at  $T/t = 0.1$  as shown in Fig. 3 (a). From this data, by performing the numerical differentiation for  $D$  with respect to  $U$ , we obtain doublon susceptibility  $\chi_D = -\partial D / \partial U$ . Here, note that, even at zero temperature, the maxima of  $\chi_D$  as the function of  $U/t$  have been demonstrated to signal the Mott transitions in the finite-size Hubbard models [32]. The obtained  $\chi_D$  is shown in Fig. 3(b). By increasing  $t'$  (increasing frustration), we find that the peak values of  $\chi_D$  decrease and the peak almost vanishes around  $t'/t \sim 0.75$ . This result indicates that the critical temperature of the critical end point of the Mott transitions becomes lower by increasing the frustration and the marginal quantum critical point (MQCP) [33, 34] exists around  $t'/t \sim 0.75$ , where the critical temperature of the Mott transition becomes zero. Because of the limitation of the available system size, it is hard to make a conclusion to the fate of the finite-temperature Mott critical point. However, our results are qualitatively consistent with the mean-field calculations [34, 35] and it is plausible that the MQCP appears around  $t'/t \sim 0.75$ . We note that ground-state

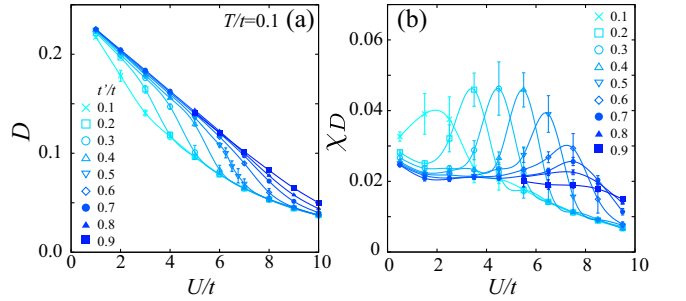


FIG. 3: (color online). (a) Interaction dependence of double occupancy  $D$  for several  $t'$  at  $T/t = 0.1$ . The crossover interaction becomes larger by increasing frustration. (b) Interaction dependence of double occupancy susceptibility  $\chi_D$  for several  $t'$ . To reduce the numerical error in numerical differentiation, we take finite difference  $\Delta U = 1$ . We see the height of peak in  $\chi_D$  becomes smaller by increasing  $t'$ . This result indicates that the critical temperature of Mott critical end point becomes lower by increasing  $t'$ .

calculations for the Hubbard model on the anisotropic triangular lattice also indicate that the Mott transitions is transformed from the first order to continuous with the increase of the geometrical frustrations signaled by the decrease in the jump of  $D$  [33, 36].

*Signatures of quantum spin liquids.*— Here, to examine the signature of the spin liquid state, we calculate spin correlations for several different  $t'$ . As shown in Fig. 4(a) and (b), in the small  $t'$  ( $t' \lesssim 0.6$ ), by lowering the temperature, antiferromagnetic nn spin correlations develop while the ferromagnetic nnn spin correlations develop. These spin correlations are consistent with the Néel order. In contrast to this, for large  $t'$  region ( $t'/t \gtrsim 0.8$ ), while the antiferromagnetic nnn spin correlations develop, the nn spin correlations remain small even at low temperatures below  $t/10$ . These spin correlations indicate that the stripe antiferromagnetic order becomes stable in the large  $t'$  region. Sandwiched by the Néel and the stripe orders,  $S_{nnn}$  is saturated and remains small even at low temperatures for the intermediate  $t'$ , which manifests suppression of magnetic orders and may indicate the spin-liquid ground states.

We next examine the thermodynamic properties of the spin-liquid candidates. In contrast to the high-temperature peaks of  $C$  insensitive to  $t'$  shown in Fig. 4(c), the positions of the second peak largely depend on  $t'$  since they are governed by the spin degrees of freedom. At the highly frustrated parameter region  $t'/t=0.75$ , the amplitude of the second peak remains small and indicates the substantial amount of low-energy excitations is left even below the energy scale  $T/t \sim 0.05$ .

To quantify the amount of the low-energy excitations, we calculate the entropy, which is defined by  $S(T)/N_s = c \ln 2 - 1/N_s \int_{-\infty}^T C/T dT$ ,  $S_{\text{norm}} = S/(c \ln 2)$ , where constant  $c$  is 2 if  $S_{\text{total}}^z$  is unrestricted. In this calculation, we set  $S_{\text{total}}^z = 0$ . Then,  $c$  is given by  $c = \ln(16C_8)^2 / 16 \ln 2 \sim 1.706$  for 16 sites. If we take the thermodynamic limit,  $c$  converges to 2. We show temperature dependence of  $S_{\text{norm}}$  in Fig 4(d). At the highly frustrated region ( $t'/t=0.75$ ), the entropy is not released down to  $T/t \sim 0.05$  compared to weakly frustrated regions.

We also show  $t'$  dependence of the entropy for several different temperature in Fig 4(e). We find that  $S_{\text{norm}}(T=t/10) \gtrsim (1/4) \times S_{\text{norm}}(T \rightarrow +\infty)$  holds within the range of the parameter  $t'/t$  corresponding to the spin-liquid or non-magnetic ground states such as valence-bond-crystal [14, 15] states at the strong coupling limit. In sharp contrast, for the Néel and stripe order, normalized entropy  $S_{\text{norm}}$  quickly becomes zero by decreasing the temperature, which indicates that almost all the degrees of freedom including spin degrees of freedom is released below  $T \sim t/10$ .

Even at the moderately high temperatures  $T \sim t/10$ , therefore, entropy  $S(T)$  clearly shows whether the target systems have chance to be spin-liquid states at zero temperature. This fact is seemingly trivial since, in the

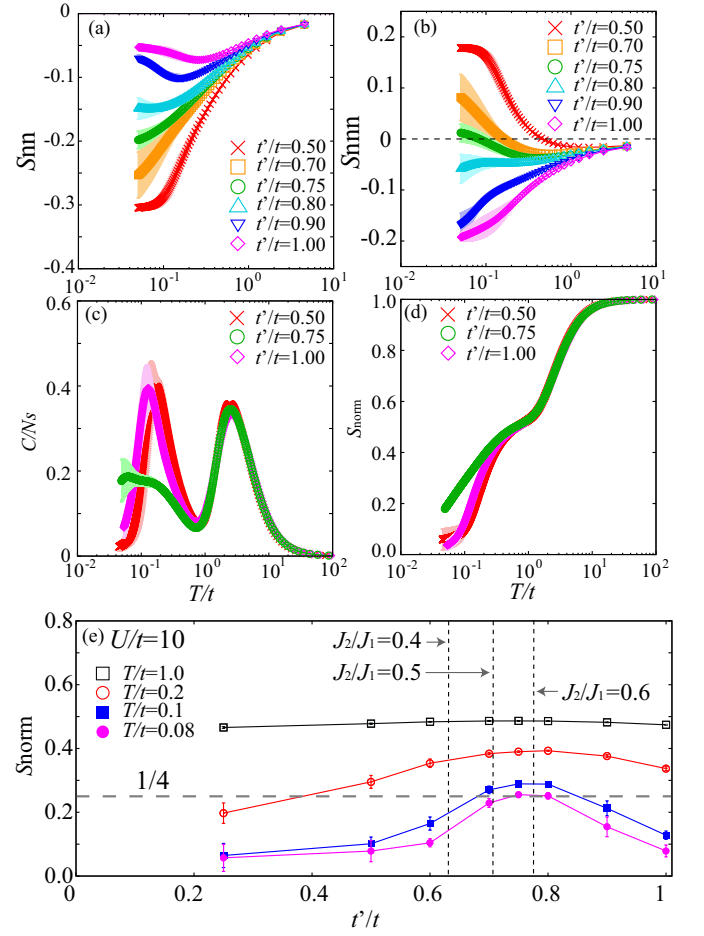


FIG. 4: (color online). (a),(b) Temperature dependence of nearest-neighbor ( $S_{nn}$ ) and next-nearest-neighbor ( $S_{nnn}$ ) spin correlations for several different  $t'$  at  $U/t = 10$ . Around  $t' \sim 0.75$ ,  $S_{nnn}$  becomes almost zero at low temperature. (c) Temperature dependence of the specific heat for several  $t'$  at  $U/t = 10$ . (d) Temperature dependence of the normalized entropy defined in main text. For  $t'/t \sim 0.75$ , large residual entropy is observed compared to  $t'/t = 0.5, 1.0$ . (e)  $t'$  dependence of the entropy for several different temperatures. Around  $t'/t \sim 0.75$ , the large remaining entropy is observed and it is the evidence of quantum spin liquid.

presence of the geometrical frustrations, entropy is expected to remain finite at low temperatures well below the exchange coupling  $J_1$ . However, the present result offers the first unbiased and quantitative criterion for the emergence of the spin-liquid ground states.

In summary, we apply the TPQ method to the frustrated Hubbard model. We show that universal double-peak structures of specific heat and non-monotonic temperature dependence of double occupancy appear in the frustrated Hubbard model. By calculating the susceptibilities of the double occupancy, we find that the characteristic energy scale of the Mott transition becomes lower by increasing  $t'$ . This result indicates emergence of the



MQCP around  $t'/t \sim 0.75$ . We also find the spin correlations are significantly suppressed around  $t'/t \sim 0.75$  and quantum spin liquid states may appear around this region. The small next-nearest-neighbor spin correlations and the large remaining entropy are the evidence of the spin-liquid states. We note that the MQCP and quantum spin liquid appear around nearly the same parameter region and we expect that this coincide is not accidental: Continuous metal-insulator transitions between paramagnetic metals with large Fermi surfaces and antiferromagnetic insulators are prohibited by the Luttinger's theorem [37]. Therefore, if a paramagnetic metal undergoes a continuous transition to an insulator in one side of MQCP, quantum spin liquid may emerge in the insulator side [38, 39]. However, it is unlikely in the strong coupling region but not excluded that the antiferromagnetic metals appear around MQCP, which are sandwiched by antiferromagnetic insulators and paramagnetic metals [34, 35]. It is an intriguing issue left for future studies to examine whether the quantum spin liquids universally appear around MQCP or not. We also offer a necessary condition on entropy [ $S(T=t/10) \gtrsim (1/4) \times S(T=+\infty)$ ] to realize a spin-liquid ground state in frustrated Hubbard models. The suppression of magnetic orders due to the low dimensionality [40] and impurities [41], instead of the geometrical frustration, is excluded by the proposed condition. For the spin liquid candidates, it is an intriguing challenge to examine whether our proposal will work.

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